

Collaborative Multi-scale Combustion Science

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A requirements white paper in support of the DOE National Collaboratory Program - January, 2005

Summary Description of Combustion Science and Community

The long-term energy security of our nation and the world presents many important fundamental science and technology challenges to the combustion research community. There is also a growing need for timely solutions driven by finite resources, and the effects of emission on human health and global climate. High efficiency, low emission processes such as Homogeneous Charge Compression Ignition (HCCI), ‘flameless combustion,’ control of soot formation and burnout, and high-pressure-ratio ultra-lean turbine combustion using fossil fuels are examples. Others involve new energy carriers such as hydrogen, and/or renewable alternative fuels that press for new knowledge of combustion interactions, dynamics and chemistry. These priorities are strongly coupled to related chemical science challenges involving catalysis, chemical processing, atmospheric chemistry, nano- and bio-chemistry and other energy storage and utilization technologies.

These challenges span, and often strongly couple, the full range of physical scales involved in combustion processes – from the properties and interactions of individual molecules to the dynamics and products of turbulent multi-phase reacting flows. This characteristic is much like that of other areas involving complex multi-scale phenomena. The situation, for example, is similar in earth system studies, fusion research, high-energy physics, and biology – an understanding of environment, device, and/or system scale phenomena requires more than simply applying one type of computation, with increased computing power, across scales. Rather, different physical phenomena dominate system dynamics at these different scales, leading to a variety of conceptual models, and associated experiments and computations, each relevant in the different regimes. Information from one regime is important input for the next, and research across multiple sub-disciplines is required to “bootstrap” the science endeavor from the atomistic to the device or system level. A counter flow of information is also critical — for validation, identifying research gaps and areas where new data will have high-impact, and identifying new application scenarios that motivate the investigation of new sub-scale processes.

There are significant unique facilities, such as highly instrumented flame facilities and high pressure combustion labs, and strong interdependencies among research issues that inspire and even require collaborative research approaches. Yet, the combustion research community is very diverse, both in its demographics and in the range of problems it addresses. It is distributed internationally with significant leadership in Europe and Japan as well as in the US and other countries. It is also encompasses a high diversity of stakeholder and sponsor agencies, with significant government and industrial involvement. In the US, for example, combustion research is supported across DOE, DOD, Commerce, NASA, and NSF. Innovative approaches to and technologies for collaboration are required to help overcome the persistent challenges arising from this extreme diversity of problems and information, including, for example, the realities of competition for recognition and sponsor funding and the often proprietary value of results to industry partners, as well as the need to integrate information across the heterogeneous and rapidly evolving set of scientific tools and supporting technologies used across the community.

Challenges, Priorities, and Requirements

In combustion research, it has long been clear that neither purely experimental, nor purely theoretical approaches will ever quantify the full range of information needed to solve our energy challenges. At the smallest scales, there is a heavy reliance on quantum theory and computations supplemented by a wide range of experimental techniques. As the molecular species grow in size, their complexity and the vast

diversity of molecular properties and reaction rates cannot yet be conquered computationally and most of the available information is from experimental techniques, though dramatic progress is being made in computational and modeling approaches. At the other end of the spectrum of scales, it is clear that *in-situ* experimental approaches will never fully resolve the finest spatial and chemical characteristics of interfacial, turbulent, and high-pressure reacting processes. At this device-scale, advanced diagnostic techniques are providing high-throughput quantitative and detailed data, providing large and valuable datasets needed by a growing collaborative modeling and simulation community.

Many of these experimental and theoretical techniques involve significant resources and require specialized expertise, and hence are supported within collaborative user facilities which face challenges associated with making their models, instruments, expertise, and data available to the broader community. At the molecular and reacting fluids scales, advanced computational implementations of models and theory are driving towards development of a multi-scale predictive understanding. Increasingly, the community is seeing their wide range of independent research efforts as contributing to a coherent hierarchy of models, computational tools, and validation experiments that will allow our society's energy challenges to be addressed much more directly and effectively.

In pursuing this goal, the combustion science community faces significant challenges integrating the information across physical scales and disciplines into validated models that span the gap between the molecular scale and that of reacting flows and combustion devices. Models encompassing reacting molecular systems, molecular transport, interfacial transport and reaction in multiphase systems, turbulence-chemistry interactions, and many more phenomena depend on theories and experiments spanning numerous disciplines. The diversity of this information and the multiplicity of institutions, agencies, and global locations from which it emanates, contribute to an 'information bottleneck' that limits the sharing of consistent, validated, and timely information among these entities. The research literature and, more recently, community databases support some level of sharing, but discovery, integration, and community evaluation and comparison of information are still tedious at best. As computational and high-throughput experimental techniques improve and mature, the information intensive processes of assembling data and software into high-quality, fully validated, well documented multiscale models is quickly becoming *the* rate-limiting step in making scientific progress.

Combustion at a Crossroads

The breadth and volume of data, experimental and computational approaches, and modeling techniques is clearly becoming sufficient to enable the community to take a systems-oriented approach to building combustion knowledge. It is also becoming clear that modern computer and information technologies can greatly facilitate such an approach. Many in the field are, in fact, already acting to develop tools and methods that will enable researchers to use systems level information to actively guide their research. Their early successes are fueling a growing enthusiasm for a more collaborative mode of combustion research. However, transforming combustion research and thereby enabling the development of powerful, predictive tools for addressing our society's energy challenges will require significant investments over the next decade. The requirements for future progress against these challenges are summarized in the sections below.

Increasing Scale of Data, Resources, and associated Tools

The increasingly large data sets (experimental and computational) and high computational requirements for this community have been documented in several DOE workshop reports [1-4].

- Currently, combustion reacting flow simulations [5] and molecular quantum chemistry computations [6] are rapidly increasing in chemical complexity and are pressing the state-of-the-art in computational resources. There is an international focus on laser-based experiments [7] and

model validation that is moving to high-throughput quantitative imaging data. Data is getting bigger fast, with requirements for collaborative analysis and data sharing capabilities that go well beyond the desktop and static HTML websites. New modes of software development enabling community-based analysis tools and MP codes are also required.

- Over the next few years, methods such as those being researched and prototyped for building modular MP codes [8], data sub-setting, feature tracking, and data sharing approaches [9] must expand and mature to enable collaborative combustion research. New tools to efficiently manage workflow for remote processes, track data and data pedigree, and collaboratively analyze data are required [3].
- By 2012, availability of ultra-scale computing resources will enable direct computation of turbulent laboratory flames, enabling direct validation of chemical and other models against experiment [2]. Computational data sets approaching 20-30 terabytes will be collaboratively defined, analyzed, and compared against complex experimental data sets. A greatly expanded database of thermochemical properties and detailed reaction rates will begin to appear from high-throughput computational approaches driven by the detailed chemistry of real fuels used in combustion applications. This not only sets a new scale for the tools needed, but also requires a new level of community involvement in the computation/evaluation of molecular properties and the development and validation of the required chemical reaction models (see next sections).

Integration of Information and associated Tools at the Speed of Science

The solution of the ‘information bottleneck’ described above requires significantly increased level of collaboration and coordination of interdisciplinary experiment planning, data acquisition, analysis, evaluation, etc. Challenges include doing this at increasing scales, lowering the time and cost barriers to include new tools, new data, new people in collaborations, and supporting interactions among a hierarchy of collaborating groups that will make up many future virtual organizations. Requirements include remote access to collaborative/shared data and analysis tools, interoperability of data, community-based evaluation of data and models, and collaborative assimilation of knowledge in information intensive chemical models.

- Currently, some combustion communities are self-organizing, using periodic workshops (e.g., ref. [7]) and static Web sites. An example of web-based community model development exists [10] but has not yet been repeated. Data is also made available by NIST [11] and others, with numerous private collections on individual web sites. New informatics approaches are being piloted [9] and are gaining broader attention. These approaches will first focus on updated reaction models spanning broader conditions for simpler fuels such as methane.
- Over the next few years, such novel informatics approaches must begin to expand to numerous communities, collectively integrating a comprehensive array of data and a large array of rapidly evolving analysis tools. Supporting molecular properties and reaction models will begin to be developed and/or updated for larger fuel surrogates such as butane and heptane. Sustainable collaborative infrastructures accessing federated data must be replicated for numerous interacting communities. Tools and support for development of community standards for namespace, metadata and schema, and data translation are needed.
- By 2012, the vision is for development and integration of new information into new models for complex chemical systems ‘on demand.’ That is, by working collaboratively across disciplines in a typical project timeframe, and based on the chemical requirements, for example, of a large scale simulation, or design of a new combustion experiment. This will require significant expansion of the role of informatics, and will require new techniques. The heterogeneity inherent in multi-scale

combustion science will require strong support for converting information between conceptual models and across formats. In addition, scalable and maintainable solutions will require increased abstraction of services and resources, while researchers will need better mechanisms to coordinate their activities within relevant groups and communities. The emerging vision for meeting these requirements is the ‘knowledge grid’ which incorporates advances being made in semantic web, informatics, collaboratory, and grid communities. Effective use of knowledge grids will also require cultural changes and iterative approaches involving long-term collaborations of domain and information researchers to fully realize the potential of cross-scale, systems-oriented informatics.

Managing Larger Collaborations and New Scientific Products

As combustion scientists begin to work more as a set of coupled collaborative communities, the record of the work must start to mirror this work approach, and the literature doesn’t suffice. So, semantically described data, standards and agreed semantic mappings between participants, provenance and annotations at a global scale, long term preservation, etc. are needed to allow knowledge grids to take on/expand upon the role of the literature for next-generation combustion science.

- Currently, some journals are offering to publish ‘supporting data’ in the chemical community, but these data bases do not support community evaluation or many other required features for community data. There is a need for recognized peer review processes for data and even applications. Some organizations, like IUPAC and NIST, traditionally involved in community evaluation, are participating in pilot efforts [9]. The NIH is already breaking some of this ground for the biomedicine community.
- Over the next few years, discussion of standards and semantic mappings, and approaches to long term preservation, etc. are needed that include major funding agencies, the publishing community, and leaders among the scientific community. New paradigms must be piloted that support publication, evaluation, and archival of scientific data and models are needed to support interdisciplinary multi-scale chemical science. The community documentation of large MP code bases and their experimental validation will also require new approaches to the publication of codes and traceable pedigree. These approaches must also consider the needs to manage intellectual property, recognize contributions, and fund community-based research and development.
- By 2012, critical information such as validated chemical and related combustion models and pedigreed molecular property data will be published and accessible for advanced ultrascale simulations and for use in designs by industry and by innovative technologists worldwide. Systems-level tools (much like that [12] being piloted now for thermochemical data) that relate a broad range of data will be required to assess the need for specific new information to support chemical models and simulations for highly complex reacting chemical systems.

A Vision for the Future of Multiscale Chemical Science

The vision of the combustion research community is to enable and build an array of predictive design tools that allow bypassing the expensive and slow ‘cut and try’ development process that fails as designs of increasingly complexity must meet conflicting requirements that press technologies to the fundamental limits imposed by nature. The predictive qualities of these tools require a vast, connected, and accessible array of computational and experimental data, validated models, and computational approaches. Such peer-reviewed, continually updated, ‘best’ models and tables will be developed and published across scales by hierarchically organized virtual organizations that thrive using stable collaborative infrastructures and global standards for sharing information. Feedback from industrial partners and new

systems-level tools that analyze sensitivities and errors will lead to requests for new inputs from other disciplines and scales. Eventually, enhanced automation of the entire sets of tools and processes will speed up this iterative process and enable the community to rapidly tackle new problems for discovery and application science.

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